CHARGE NUMBER: 2515

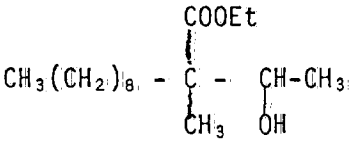
PROJECT TITLE: Flavor-Release Chemistry

PROJECT LEADER: Yoram Houminer

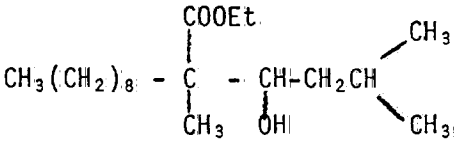
PERIOD COVERED: February 1-28, 1983

DATE OF REPORT: March 9, 1983

We are continuing our research in the area of aldehyde release. Ethyl 2-(1-hydroxyethyl)-2-methylundecanoate (I) was prepared in 59% yield by reacting the enolate anion of ethyl 2-methylundecanoate with acetaldehyde.[1] The hydroxy-ester derivative of isovaleraldehyde (II) was obtained by a similar procedure.[2] In both cases, the products are mixtures of two diastereoisomers in about 1:1 ratio.



I

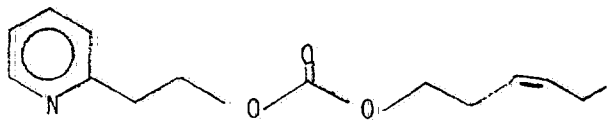


II

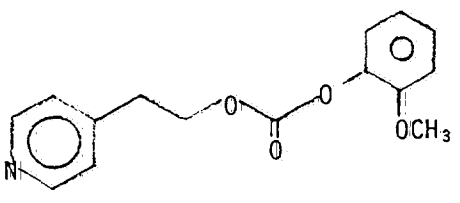
Pyrolysis of I at 300°C for 1 min. under a flow of hellium yielded 18% of acetaldehyde. At 400°C, a quantitative yield of acetaldehyde was obtained.[3] Pyrolysis of II at 250°C for 5 min. in an open tube gave 45% release of isovaleraldehyde. We plan to further explore the potential of these systems as precursors for low molecular weight aldehydes.

All eight possible isomers of phenyl aldopentopyranosides (the α and β-anomers of arabino-, lyxo-, ribo- and xylopyranosides) were purified.[1] Conformational analysis by NMR will be carried out, and we hope that such information will provide insight on the mechanism of the aryl glycosidation reaction.

We are continuing our study in the area of carbonates derived from pyridylethanols and a variety of phenols and alcohols. Compound III and IV were prepared by reacting the corresponding pyridylethanol with the corresponding chloroformate.[4]



III



IV

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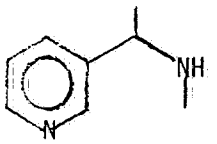
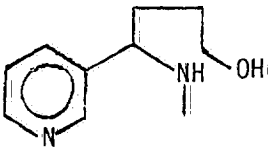
Pyrolysis of III at 250°C for 10 min. gave only 5% of the desired cis-3-hexenol, whereas the phenyl analogue of III has been shown to give >50% of phenol under similar conditions. These results indicate that carbonates derived from 2-pyridylethanol are good precursors for phenolic flavorants but not for alcohols.[4] Pyrolysis of carbonates of the 4-pyridyl isomer will be carried out in the near future.

We have successfully prepared the amine V by reacting 3-acetylpyridine with methylamine in the presence of $NaCNBH_3$. This methodology will be applied in the preparation of VI, a precursor designed to release nicotine.[4]



V



VI

We have completed the analysis of levels of CR-1845 on cigarettes that were fabricated for smoking studies. Our five-port smoking machine was recently refurbished and preliminary smoking experiments are now in progress.[5]

A patent disclosure entitled "Dicarbonates of 2,5-dihydroxy-1,4-dioxane as release agents for alcohol and phenol flavorants" by K. F. Podraza was submitted to the patent department. A manuscript entitled "Stereoselective synthesis of aryl aldopyranosides" was submitted to MRB by G. Chan.

References

1. G. Chan, 7734
2. Y. Houminer, 7747
3. Carried out by L. Brown
4. K. Podraza, 7851
5. J. Kang, 7692

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